

L Number	Hits	Search Text	DB	Time stamp
1	3715	(436/173,174,2,86,94,95).CCLS.	USPAT; US-PGPUB; EPO, JPO; DERWENT	2004/01/05 18:50
2	44	((436/173,174,2,86,94,95).CCLS.) and (isotop\$3 near3 ratio\$2)	USPAT; US-PGPUB; EPO, JPO; DERWENT	2004/01/05 18:50
-	2	"200079569"	USPAT; US-PGPUB; EPO, JPO; DERWENT	2004/01/05 18:47
-	13	"2120007"	USPAT; US-PGPUB; EPO, JPO; DERWENT	2003/12/18 17:19
-	0	NMR-FINS	USPAT; US-PGPUB; EPO, JPO; DERWENT	2003/12/18 17:25
-	0	NMR near2 SNIF	USPAT; US-PGPUB; EPO, JPO; DERWENT	2003/12/18 17:26
-	53	(isotop\$2 near3 (ratio\$2 or distribution\$2)) with (mass near2 spectr\$5)	USPAT; US-PGPUB; EPO, JPO; DERWENT	2003/12/19 14:45
-	40	((isotop\$2 near3 (ratio\$2 or distribution\$2)) with (mass near2 spectr\$5)) and referenc\$2	USPAT; US-PGPUB; EPO, JPO; DERWENT	2003/12/22 11:00
-	18	(isotop\$2 near3 (ratio\$2 or distribution\$2)) with (authent\$5 or origin or freud)	USPAT; US-PGPUB; EPO, JPO; DERWENT	2003/12/22 11:01

FILE 'CAPLUS' ENTERED AT 12:28:50 ON 22 DEC 2003

L1 914 (ISOTOP? (3A) (RATIO? OR DISTRIBUTION?)) (S) (AUTHENT? OR ORIGIN OR FREUD?)

L2 0 L1 AND (MASS (3A) SPCTR?)

L3 214 L1 AND (MASS (3A) SPECTR?)

L4 35 L3 AND NMR

L5 53 L3 AND (FRAGMENT? OR CLEAV? OR PRODUCT? OR RAW)

L6 2 L1 AND (FRAGMENTATION OR CLEAVAGE)

L4 ANSWER 1 OF 35 CAPLUS COPYRIGHT 2003 ACS on STN

TI Official methods based on stable isotope techniques for analysis of food. Ten years' of European experience

L4 ANSWER 2 OF 35 CAPLUS COPYRIGHT 2003 ACS on STN

TI Characterization of animal products according to geographic origin and feeding diet using nuclear magnetic resonance and isotope ratio mass spectrometry: cow milk

L4 ANSWER 3 OF 35 CAPLUS COPYRIGHT 2003 ACS on STN

TI Authentication of tequila by gas chromatography and stable isotope ratio analyses

L4 ANSWER 4 OF 35 CAPLUS COPYRIGHT 2003 ACS on STN

TI Possibilities and limitations of wine authentication using stable isotope and meteorological data, Data banks and statistical tests. Part 1: Wines from Franconia and Lake Constance 1992 to 2001

L4 ANSWER 5 OF 35 CAPLUS COPYRIGHT 2003 ACS on STN

TI Food chemistry 2002

L4 ANSWER 6 OF 35 CAPLUS COPYRIGHT 2003 ACS on STN

TI Multielement, multicomponent, and multisite isotopic profiling for food and beverage authentication

L4 ANSWER 7 OF 35 CAPLUS COPYRIGHT 2003 ACS on STN

TI Isotope fingerprinting: tracing the origin of products

L4 ANSWER 8 OF 35 CAPLUS COPYRIGHT 2003 ACS on STN

TI Stable isotope abundance and pattern analysis - a potent tool in flavour origin and authenticity control

L4 ANSWER 9 OF 35 CAPLUS COPYRIGHT 2003 ACS on STN

TI High precision isotope ratio fingerprinting of ethanol and other commercial molecules and materials

L4 ANSWER 10 OF 35 CAPLUS COPYRIGHT 2003 ACS on STN

TI Determination of Authenticity, Regional Origin, and Vintage of Slovenian Wines Using a Combination of IRMS and SNIF-NMR Analyses

L4 ANSWER 11 OF 35 CAPLUS COPYRIGHT 2003 ACS on STN

TI Use of SNIF-NMR and IRMS in combination with chemometric methods for the determination of chaptalization and geographical origin of wines (the example of Slovenian wines)

L4 ANSWER 12 OF 35 CAPLUS COPYRIGHT 2003 ACS on STN

TI Analysis of oxygen-18 in orthophosphate by electrospray ionization mass spectrometry

- L4 ANSWER 13 OF 35 CAPLUS COPYRIGHT 2003 ACS on STN
TI High precision position-specific isotope analysis
- L4 ANSWER 14 OF 35 CAPLUS COPYRIGHT 2003 ACS on STN
TI Multielement IRMS of flavor compounds
- L4 ANSWER 15 OF 35 CAPLUS COPYRIGHT 2003 ACS on STN
TI Incorporation of ^{13}C -labeled coniferyl alcohol into developing Ginkgo biloba L. lignin revealed by analytical pyrolysis and CuO oxidation in combination with isotope ratio monitoring-gas chromatography-mass spectrometry
- L4 ANSWER 16 OF 35 CAPLUS COPYRIGHT 2003 ACS on STN
TI Site-specific isotope effects and origin inference
- L4 ANSWER 17 OF 35 CAPLUS COPYRIGHT 2003 ACS on STN
TI Stable oxygen isotope content of water of EU data-bank wines from Italy, France, and Germany
- L4 ANSWER 18 OF 35 CAPLUS COPYRIGHT 2003 ACS on STN
TI Quantitative isotopic NMR of quadrupolar and dipolar nuclei
- L4 ANSWER 19 OF 35 CAPLUS COPYRIGHT 2003 ACS on STN
TI Use of Isotopic Analyses To Determine the Authenticity of Brazilian Orange Juice (Citrus sinensis)
- L4 ANSWER 20 OF 35 CAPLUS COPYRIGHT 2003 ACS on STN
TI Authenticity assessment of flavors and fragrances
- L4 ANSWER 21 OF 35 CAPLUS COPYRIGHT 2003 ACS on STN
TI Assignment of raw material and authentication of spirits by gas chromatography, hydrogen-, and carbon-isotope ratio measurements. Part 1. Analytical methods and results of a study of commercial products
- L4 ANSWER 22 OF 35 CAPLUS COPYRIGHT 2003 ACS on STN
TI Application of ^2H SNIF-NMR and ^{13}C SIRA-MS Analyses to Maple Syrup: Detection of Added Sugars
- L4 ANSWER 23 OF 35 CAPLUS COPYRIGHT 2003 ACS on STN
TI Interpretation of combined ^2H SNIF/NMR and ^{13}C SIRA/MS analyses of fruit juices to detect added sugar
- L4 ANSWER 24 OF 35 CAPLUS COPYRIGHT 2003 ACS on STN
TI Enantioselectivity and isotope discrimination as biogenetic fixed parameter for natural flavors and fragrances
- L4 ANSWER 25 OF 35 CAPLUS COPYRIGHT 2003 ACS on STN
TI Search for chlorinated sesquiterpene lactones in the neurotoxic thistle Centaurea solstitialis by liquid chromatography-mass spectrometry, and model studies on their possible artifactual formation
- L4 ANSWER 26 OF 35 CAPLUS COPYRIGHT 2003 ACS on STN
TI Novel triterpene-derived hydrocarbons of the arborane/fernane series in sediments: Part II
- L4 ANSWER 27 OF 35 CAPLUS COPYRIGHT 2003 ACS on STN
TI Deuterium, carbon and nitrogen isotopic analysis of natural and synthetic caffeine. Authentication of coffees and coffee extracts
- L4 ANSWER 28 OF 35 CAPLUS COPYRIGHT 2003 ACS on STN
TI A coupled NMR and MS isotopic method for the authentication of natural vinegars
- L4 ANSWER 29 OF 35 CAPLUS COPYRIGHT 2003 ACS on STN

TI Authentication of essential oils containing linalool and linalyl acetate by isotopic methods

L4 ANSWER 30 OF 35 CAPLUS COPYRIGHT 2003 ACS on STN

TI Combination of mass spectrometry and site-specific NMR isotope analyses in the characterization of amino acids

L4 ANSWER 31 OF 35 CAPLUS COPYRIGHT 2003 ACS on STN

TI Determination of site-specific carbon isotope ratios at natural abundance by carbon-13 nuclear magnetic resonance spectroscopy

L4 ANSWER 32 OF 35 CAPLUS COPYRIGHT 2003 ACS on STN

TI Authentication of fragrances and perfumes by nuclear magnetic resonance and isotope-ratio mass spectrometry.

L4 ANSWER 33 OF 35 CAPLUS COPYRIGHT 2003 ACS on STN

TI Food quality control and studies on human nutrition by mass spectrometric and nuclear magnetic resonance isotope ratio determination

L4 ANSWER 34 OF 35 CAPLUS COPYRIGHT 2003 ACS on STN

TI A new method for the identification of the origin of natural products. Quantitative deuterium NMR at the natural abundance level applied to the characterization of anetholes

L4 ANSWER 35 OF 35 CAPLUS COPYRIGHT 2003 ACS on STN

TI Use of carbon-13 in biosynthetic studies. The labeling pattern in tenellin enriched from isotope-labeled acetate, methionine, and phenylalanine

L4 ANSWER 7 OF 35 CAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 2003:62025 CAPLUS

DOCUMENT NUMBER: 139:5784

TITLE: *"Isotope fingerprinting: tracing the origin of products"*

AUTHOR(S): *Martin, Maryvonne L.; Martin, Gerard J.*

CORPORATE SOURCE: *Universite de Nantes, Eurofins Scientific, Nantes, 44323, Fr.*

SOURCE: *Comptes Rendus de l'Academie d'Agriculture de France (2001), 87(8), 41-46*

CODEN: CRAFEQ; ISSN: 0989-6988

PUBLISHER: *Academie d'Agriculture de France*

DOCUMENT TYPE: *Journal; General Review*

LANGUAGE: *French*

AB A review discussing the use of techniques such as isotope ratio mass spectrometry (IRMS) and site-specific natural isotope fractionation by NMR (SNIF-NMR) to assess the origin of food and other natural products. The isotopic fingerprint contains information concerning not only the nature of the precursors and the mechanisms of chem. or biochem. synthesis, but also changes in environmental conditions. When compared to traditional authentication criteria, which are based on compositional data, the isotopic parameters are more robust, they are more rigorously interpretable on a theor. basis, and they can be applied to assess the origin of pure mol. species.

REFERENCE COUNT: 3

L4 ANSWER 8 OF 35 CAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 2001:554381 CAPLUS

DOCUMENT NUMBER: 136:84823

TITLE: "Stable isotope abundance and pattern analysis – a potent tool in flavour origin and authenticity control"

AUTHOR(S): *Rossmann, A.; Schmidt, H.-L.*

CORPORATE SOURCE: Lehrstuhl für Biologische Chemie der Technischen Universität München, Freising-Weihenstephan, 85350, Germany

SOURCE: Frontiers of Flavour Science, [Proceedings of the Weurman Flavour Research Symposium], 9th, Freising, Germany, June 22-25, 1999 (2000), Meeting Date 1999,97-101. Editor(s): Schieberle, Peter; Engel, Karl-Heinz. Deutsche Forschungsanstalt für Lebensmittelchemie: Garching, Germany.

CODEN: 69BOX5

DOCUMENT TYPE: Conference; General Review

LANGUAGE: English

AB A review with refs. Principles and possibilities of stable isotope ratio anal. (SIRA) for flavor substances origin assignment, as performed applying isotope ratio mass spectrometry (IRMS) and/or NMR spectroscopy (NMR) are described. After a discussion of advantages and disadvantages of both methods, typical applications are described. The use of intermol. and intramol. ref. methods and of multielement isotopic data is demonstrated. For the future, the necessity of extended basic research, esp. regarding nitrogen and sulfur isotopes, the compilation of databases for substances of defined origin, and even further instrumental improvements are outlined.

REFERENCE COUNT: 30

L4 ANSWER 10 OF 35 CAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 2001:91804 CAPLUS

DOCUMENT NUMBER: 134:294726

TITLE: Determination of Authenticity, Regional Origin, and Vintage of Slovenian Wines Using a Combination of IRMS and SNIF-NMR Analyses

AUTHOR(S): Ogrinc, Nives; Kosir, Iztok J.; Kocjancic, Mitja; Kidric, Jurkica

CORPORATE SOURCE: Department of Environmental Sciences, J. Stefan Institute, Ljubljana, 1000, Slovenia

SOURCE: Journal of Agricultural and Food Chemistry (2001), 49(3), 1432-1440

CODEN: JAFCAU; ISSN: 0021-8561

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The authenticity and geog. origin of wines produced in Slovenia were investigated by a combination of IRMS and SNIF-NMR methods. A total of 102 grape samples of selected wines were carefully collected in 3 different wine-growing regions of Slovenia in 1996, 1997, and 1998. The stable isotope data were evaluated using principal component anal. (PCA) and linear discriminant anal. (LDA). The isotopic ratios to discriminate between coastal and continental regions are the deuterium/hydrogen isotopic ratio of the methylene site in the ethanol mol. (D/H)II and $\delta^{13}\text{C}$ values; including also $\delta^{18}\text{O}$ values in the PCA and LDA made possible sepn. between the 2 continental regions Drava and Sava. It was found that $\delta^{18}\text{O}$ values are modified by the meteorol. events during grape ripening and harvest. The usefulness of isotopic

parameters for detecting adulteration or watering and to assess the geog. origin of wines is improved only when they are used concurrently. REFERENCE COUNT: 34

L4 ANSWER 11 OF 35 CAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 2001:70839 CAPLUS

DOCUMENT NUMBER: 134:279740

TITLE: Use of SNIF-NMR and IRMS in combination with chemometric methods for the determination of chaptalization and geographical origin of wines (the example of Slovenian wines)

AUTHOR(S): Kosir, I. J.; Kocjancic, M.; Ogrinc, N.; Kidric, J.

CORPORATE SOURCE: National Institute of Chemistry, Ljubljana, 1000, Slovenia

SOURCE: *Analytica Chimica Acta* (2001), 429(2), 195-206

CODEN: ACACAM; ISSN: 0003-2670

PUBLISHER: Elsevier Science B.V.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Isotopic ratios detd. by SNIF-NMR and IRMS methods were used in combination with chemometric methods PCA, KANN and cluster anal. for the detection of wine chaptalization and differentiation of wines according to the geog. origin. Selected wines from the three wine-growing regions of Slovenia were chosen for the anal. since Slovenia, small by surface, but pedol. and climatically diverse, offers possibilities for studying the influence of this diversity upon the isotopic ratios in mols. of natural products. We found that the sepn. of wines of the Coastal region from the wines of the continental regions Sava and Drava is very good. On the other hand, the sepn. between wines from the Sava and the Drava region is not satisfactory. This is not surprising since the climatic differences between these two regions are small, when compared with the differences between the continental and Coastal regions. Regarding the chaptalization, e improvement by combining both SNIF- NMR and IRMS is obtained. PCA and KANN give comparable sepn. of wines according to the geog. origin, but PCA is less time consuming. In the case of enrichment of wines from the Drava region by beet sugar, better sepn. between natural and enriched wines is obtained using the KANN method. In all cases cluster anal. shows poorer efficiency than PCA and KANN.

REFERENCE COUNT: 20

L4 ANSWER 13 OF 35 CAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 2000:549973 CAPLUS

DOCUMENT NUMBER: 133:290480

TITLE: "High precision position-specific isotope analysis"

AUTHOR(S): Brenna, J. Thomas; Corso, Thomas N.

CORPORATE SOURCE: Division of Nutritional Sciences, Cornell University, Ithaca, NY, 14853, USA

SOURCE: *Synthesis and Applications of Isotopically Labelled Compounds 1997, Proceedings of the International Symposium, 6th, Philadelphia, PA, United States, Sept. 14-18, 1997 (1998), Meeting Date 1997, 115-117. Editor(s): Heys, J. Richard; Melillo, David G. John Wiley & Sons Ltd.: Chichester, UK.*

CODEN: 69AGFQ

DOCUMENT TYPE: Conference

LANGUAGE: English

AB Intramol. C distributions are normally detd. at low precision, requiring high levels of labeling to enable anal. by conventional org. mass spectrometry or NMR. Studies targeted at detn. of intramol. C isotope concns. or ratios due to natural processes were undertaken to reveal the origin of org. compds. and provide insight on the status of complex systems, such as environmental or physiol. state. Such studies require very high precision to detect small changes and have always required laborious chem. degrdn. and sepn. steps prior to isotope ratio mass spectrometry (IRMS) anal. A strategy is reported here for online continuous-flow (CF) high-precision detn. of $^{13}\text{C}/^{12}\text{C}$ ratios at specific positions in org. compds. Analyte sepd. from complex mixts. can be probed at very high sensitivity for artificially labeled positions or for variability due to natural process.

REFERENCE COUNT: 2

L4 ANSWER 14 OF 35 CAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 2000:341892 CAPLUS

TITLE: "Multielement IRMS of flavor compounds"

AUTHOR(S): *Schmidt, C. O.; Krammer, G. E.; Gatfield, I.; Hilmer, J.-M.; Sommer, H.; Meier, L.; Herbrand, K.; Werkhoff, P.*

CORPORATE SOURCE: Corporate Research, Haarmann and Reimer GmbH, Holzminden, 37603, Germany

SOURCE: **Isotopes in Environmental and Health Studies (1999), 35(4), 275**

CODEN: IEHSF8; ISSN: 1025-6016

PUBLISHER: Gordon & Breach Science Publishers

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The technique of isotope ratio mass spectrometry (IRMS) reveals the stable isotope ratios of the bioelements C, H, O, N, and S in various compds. The technique is widely used for authenticity verification of flavor compds. [1] but also for many other applications like biosynthesis elucidation and geol. chem. The anal. of the stable isotope ratios ($\delta^{13}\text{C}$, $\delta^2\text{H}$, $\delta^{18}\text{O}$, $\delta^{15}\text{N}$, $\delta^{34}\text{S}$ values) give information about the origin of a sample. In addn. to IRMS, positional isotope anal. can be performed by site specific NMR (SNIF-NMR) [2]. The detn. of stable isotope ratios of org. compds. from plants gives insight in the biochem. pathways used by the plant. Three major pathways for the CO_2 -fixation are known for plants [3]. So called C3 plants (e.g., wheat, barley, sugar beet) use the ribulosebisphosphate-carboxylase reaction (Calvin pathway), while C4 plants (e.g., sugar cane, corn) use the phosphoenolpyruvate-carboxylase reaction (Hatch-Slack pathway); CAM plants like succulents and orchids (e.g., vanilla planifolia) have the crassulacean acid metab. Each group shows different $\delta^{13}\text{C}$, $\delta^2\text{H}$, and $\delta^{18}\text{O}$ values for their metabolites as shown by IRMS (e.g., carbohydrates, secondary metabolites). Addnl., it is possible to distinguish between compds. produced by plant and synthetically produced substances. To det. the origin of a compd., i.e., from which source it is synthesized, IRMS is used in different approaches. Opposite to the older off-line detn. of stable isotope ratios, the online technique provides a coupling of a GC to the IRMS system using a combustion reactor interface (GC-IRMS) [4]. Therefore, even individual compds. in a complex mixt. could be analyzed.

However, non-volatile compds. are not suited for GC anal., those substances are applied to an IRMS system by methods of elemental anal. (for instance the TC/EA-IRMS system from Finnigan). Our work deals with the online detn. of $\delta^{13}\text{C}$, $\delta^2\text{H}$, $\delta^{18}\text{O}$ and $\delta^{15}\text{N}$ values of flavor compds. by using GC-IRMS and EA-IRMS.

REFERENCE COUNT: 6

L4 ANSWER 16 OF 35 CAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1999:503263 CAPLUS

DOCUMENT NUMBER: 131:268685

TITLE: "Site-specific isotope effects and origin inference"

AUTHOR(S): *Martin, M. L.; Martin, G. J.*

CORPORATE SOURCE: Site de la Geraudiere, CEAIS, Nantes, 44323, Fr.

SOURCE: *Analusis* (1999), 27(3), 209-213

CODEN: ANLSCY; ISSN: 0365-4877

PUBLISHER: EDP Sciences

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The isotope contents existing at natural abundance are governed by a complex set of parameters linked to both synthetic and biosynthetic mechanisms and to environmental conditions. Whereas isotope ratio mass spectrometry (IRMS) precisely measures the overall isotope content of a mol. species, NMR enables site-specific natural isotope fractionation to be studied (SNIF-NMR). From a fundamental point of view the isotopic pattern of a given mol. is a rich source of information on the reaction pathway and in particular on the genealogy of the atoms, on the relative rates of certain reaction steps, on the percentages of intra- and inter-mol. hydrogen transfer and possibly on the stereospecificity of the reactions. Consequently it is not surprising that the natural abundance isotope ratios provide powerful anal. criteria for authenticating the origin of products. Used either alone, or combined with IRMS, the SNIF-NMR method is capable of unambiguously characterizing an increasing no. of products in terms of synthetic or natural origin, botanical nature of the plant precursor, geog. origin and, sometimes, year of prodn. Many applications in the fields of fruit juices, wines and alc. beverages, aromas, oils, and drugs have now been developed. REFERENCE COUNT: 40

L4 ANSWER 19 OF 35 CAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1998:221384 CAPLUS

DOCUMENT NUMBER: 128:204196

TITLE: "Use of Isotopic Analyses To Determine the Authenticity of Brazilian Orange Juice (*Citrus sinensis*)"

AUTHOR(S): *Pupin, A. M.; Dennis, M. J.; Parker, I.; Kelly, S.; Bigwood, T.; Toledo, M. C. F.*

CORPORATE SOURCE: Centro Pluridisciplinar de Pesquisas Quimicas Biologicas e Agricolas (CPQBA), Universidade Estadual de Campinas, Campinas, 13081-970, Brazil

SOURCE: *Journal of Agricultural and Food Chemistry* (1998), 46(4), 1369-1373

CODEN: JAFCAU; ISSN: 0021-8561

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Isotopic anal. was used to characterize authentic samples of orange juice (*Citrus sinensis*) from Brazil. Site specific natural isotopic fractionation NMR (SNIF-NMR) was used to det. deuterium/hydrogen ratios at the Me [(D/H)I] and methylene [(D/H)II] sites of ethanol produced by fermn. of orange juice. Stable isotope ratio mass spectrometry (SIRMS) was used to det. the ratio of carbon isotopes ($^{13}\text{C}/^{12}\text{C}$) in the same ethanol and the ratio of oxygen isotopes ($^{18}\text{O}/^{16}\text{O}$) in the citrus juice water. The mean ratios found for these parameters in authentic hand-squeezed orange juice were as follows: (D/H)I, 102.3 ppm (SD = 1.7); (D/H)II, 126.5 ppm (SD = 1.8); $^{13}\text{C}/^{12}\text{C}$, $\delta^{13}\text{C} = -26.6$ permill. PDB (SD = 0.9); and $^{18}\text{O}/^{16}\text{O}$, $\delta^{18}\text{O} = +2.27$ permill. SMOW (SD = 2.48). Retail samples taken from the Brazilian market place were evaluated by comparison against these data. No evidence was found for the addn. of sugar to orange juice or for the diln. with tap water of samples labeled as freshly squeezed.

REFERENCE COUNT: 19

L4 ANSWER 20 OF 35 CAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1998:145249 CAPLUS

DOCUMENT NUMBER: 128:216455

TITLE: "Authenticity assessment of flavors and fragrances"

AUTHOR(S): *Mosandl, A.; Dietrich, A.; Faber, B.; Frank, C.; Juchelka, D.; Karl, V.; Lehmann, D.; Maas, B.; Weber, B.*

CORPORATE SOURCE: Institut für Lebensmittelchemie, Johann Wolfgang Goethe-Universität, Frankfurt/Main, 60439, Germany

SOURCE: **Current Status and Future Trends in Analytical Food Chemistry, Proceedings of the European Conference on Food Chemistry, 8th, Vienna, Sept. 18-20, 1995 (1995), Volume 1, 79-84.** Editor(s): Sontag, Gerhard; Pfannhauser, Werner. Austrian Chemical Society: Vienna, Austria.

CODEN: 65SOA5

DOCUMENT TYPE: Conference; General Review

LANGUAGE: English

AB A review with 17 refs. Both phenomena, enantioselectivity as well as isotope discrimination during biosynthesis may serve as endogenetic parameters in the authenticity control of natural flavor and fragrance compds., if suitable methods and comprehensive data from authentic sources are available. Besides site specific natural isotope fractionation, measured by NMR-spectroscopy (SNIF-NMR) enantioselective capillary gas chromatog. (enantio-cGC) and comparative isotope ratio mass spectrometry (IRMS), coupled online with cGC have proved to be highly efficient tools in the origin specific anal. and authenticity control of flavor and fragrance compds.

REFERENCE COUNT: 17

L4 ANSWER 22 OF 35 CAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1996:583990 CAPLUS

DOCUMENT NUMBER: 125:245875

TITLE: "Application of ^2H SNIF-NMR and ^{13}C SIRA-MS Analyses to Maple Syrup: Detection of Added Sugars"

AUTHOR: *Martin, Gilles G.; Martin, Yves-Loic; Naulet, Norbert; McManus, Hugh J. D.*

CORPORATE SOURCE: Eurofins, Nantes, 44073, Fr.

SOURCE: **Journal of Agricultural and Food Chemistry** (1996), 44(10), 3206-3213

CODEN: JAFCAU; ISSN: 0021-8561

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The SNIF-NMR method may be used to measure the site specific isotope concns. in a variety of org. compds. The most common application of this technique involves quant. deuterium NMR spectroscopy with appropriate interpretation of the accumulated spectra. SNIF- NMR together with SIRA-MS provides a powerful tool for food authentication and characterization. The concerted use of SNIF- NMR (deuterium) and SIRA-MS (carbon-13) on ethanol fermented from sugars has proven invaluable to the authentication of wines, spirits, and fruit juices. In this work, the anal. is extended to the authentication of maple syrup, a product rich in sucrose. Authentic maple syrup samples have been analyzed in detail to characterize the intrinsic variability of the isotopic ratios in this product. These data constitute a data base of authentic samples to which an unknown example of maple syrup can be compared. The isotopic ratios obtained from maple syrup are very different from those of both beet and cane or corn sugars. Therefore, the methodologies developed in this work are applicable for the detection of beet and cane or corn sugar added to a maple syrup. It can be shown that, through a simple statistical comparison between the data base and the unknown, a detn. of the occurrence and/or extent of adulteration with added sugar can be made.

L4 ANSWER 23 OF 35 CAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1996:155230 CAPLUS

DOCUMENT NUMBER: 124:230341

TITLE: Interpretation of combined 2H SNIF/NMR and 13C SIRA/MS analyses of fruit juices to detect added sugar

AUTHOR(S): Martin, Gilles G.; Hanote, Valerie; Lees, Michele; Martin, Yves-Loic

CORPORATE SOURCE: Site de la Geraudiere, ERROFINS, Nantes, 03, Fr.

SOURCE: **Journal of AOAC International** (1996), 79(1), 62-72

CODEN: JAINEE; ISSN: 1060-3271

PUBLISHER: AOAC International

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The site-specific natural isotopic fractionation studied by NMR (SNIF/NMR) method measures site-specific isotope contents in a variety of org. compds. by deuterium NMR spectroscopy. This technique, together with SIRA/MS (stable isotope ratio anal./mass spectrometry) provides a powerful tool for food authentication and characterization. By using the ethanol resulting from sugar fermn. as a mol. probe, SNIF/NMR (deuterium) and SIRA/MS (13C) have been used together for authentication of fruit juices. The influence of deuterium content of the fermn. water on the isotopic parameters is shown and a means for normalizing the results is proposed. A large no. of authentic juices have been analyzed to define the variation of isotopic ratios in natural juices. On the basis of these data, a set of rules was designed to enable interpretation of isotopic parameters in terms of possible adulteration of fruit juices by sugar addn.

Results of analyses of Florida orange juice are presented. Orange juice samples from Brazil and Israel are included as 2 extreme cases. Assignment limits for a sample of orange juice of unknown origins also are given. These assignment limits are also provided for apple and grapefruit juices.

L4 ANSWER 24 OF 35 CAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1995:982096 CAPLUS

DOCUMENT NUMBER: 124:143778

TITLE: Enantioselectivity and isotope discrimination as biogenetic fixed parameter for natural flavors and fragrances

AUTHOR(S): Mosandl, A.

CORPORATE SOURCE: Inst. Lebensmittelchem., Johann Wolfgang Goethe-Univ., Frankfurt/Main, D-60439, Germany

SOURCE: Lebensmittelchemie (1995), 49(6), 130-3

CODEN: LEBEE2; ISSN: 0937-1478

PUBLISHER: VCH

DOCUMENT TYPE: Journal; General Review

LANGUAGE: German

AB A review with 9 refs. on the origin assessment of the of natural flavors and fragrances for foods and perfumes by isotope ratio mass spectrometry, isotope fractionation NMR, enantioselective capillary gas chromatog., or combined methods.

L4 ANSWER 27 OF 35 CAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1992:192922 CAPLUS

DOCUMENT NUMBER: 116:192922

TITLE: "Deuterium, carbon and nitrogen isotopic analysis of natural and synthetic caffees. Authentication of coffees and coffee extracts"

AUTHOR(S): *Danho, D.; Naulet, N.; Martin, G. J.*

CORPORATE SOURCE: Lab. Reson. Magn. Nucl. React. Chim., CNRS, Nantes, 44072, Fr.

SOURCE: *Analusis* (1992), 20(3), 179-84

CODEN: ANLSCY; ISSN: 0365-4877

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Isotope ratio mass spectrometry (IRMS) was used to det. the .delta.(13C) and .delta.(15N) values of a series of caffeine samples extd. from coffee beans or obtained by synthesis; 2H NMR spectra were recorded to compute the site-specific isotope ratios of caffeine. The set of the five isotope ratios measured for the 26 different samples was studied by multivariate anal. (principal component and discriminant analyses), and it was shown that the synthetic samples are clearly distinguishable from the natural caffeine which in turn can be classified with complete accuracy as of either American or African origin.

L4 ANSWER 28 OF 35 CAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1992:172552 CAPLUS

DOCUMENT NUMBER: 116:172552

TITLE: A coupled NMR and MS isotopic method for the authentication of natural vinegars

AUTHOR(S): Remaud, Gerald; Guillou, Claude; Vallet, Claude; Martin, Gerard J.

CORPORATE SOURCE: Eurofins S. A., Nantes, F-44073, Fr.

SOURCE: Fresenius' Journal of Analytical Chemistry (1992), 342(4-5), 457-61

CODEN: FIACES; ISSN: 0937-0633

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The natural site-specific $2H$ content and the overall $13C$ content of acetic acid extd. from vinegars or obtained by chem. synthesis were detd. by NMR and mass spectrometries. The isotope ratios $(D/H)CH_3$ and the $\delta^{13}C$ deviation of these samples were compared to those of EtOH of the same natural or synthetic origins. The different groups of natural and fossil acetic acids are represented in the $2H/13C$ isotopic plane and the discriminant function, which enables unknown samples to be assigned to a given group, is computed. A careful anal. of the repeatability of the entire anal. procedure and a study of known mixts. of natural and synthetic acids show that as low as 5% synthetic acid in a natural vinegar can be detected in a comparative anal. A sensitivity level of 15% may be expected on an abs. basis when no information on the origin of the precursors is available, providing that a detn. of the botanical family of the natural component can be carried out beforehand.

L4 ANSWER 29 OF 35 CAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1992:46005 CAPLUS

DOCUMENT NUMBER: 116:46005

TITLE: "Authentication of essential oils containing linalool and linalyl acetate by isotopic methods"

AUTHOR *Hanneguelle, Sophie; Thibault, Jean Noel; Naulet, Norbert; Martin, Gerard J.*

CORPORATE SOURCE: Lab. RMN React. Chim., CNRS, Nantes, F-44072, Fr.

SOURCE: **Journal of Agricultural and Food Chemistry (1992), 40(1), 81-7**

CODEN: JAFCAU; ISSN: 0021-8561

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Site-specific natural isotope fractionation studied by NMR (SNIF NMR) combined with mol. isotope ratio detn. by mass spectrometry (IRMS) was used to characterize linalool and linalyl acetate obtained from chem. synthesis or extd. from essential oils of well-defined botanical and geog. origins. In general, the overall carbon-13 or deuterium contents measured by IRMS do not constitute efficient criteria for identifying natural and synthetic samples. In contrast, the nonrandom distribution of deuterium exhibits large variations as a function of the origin of the sample. A discriminant anal. performed in a space defined by the 10 site-specific hydrogen isotope ratios and the overall carbon isotopic parameter enables the natural and synthetic species to be unambiguously distinguished. In spite of the relatively large dispersion of the isotope ratios exhibited by both natural and synthetic families, it is possible to develop an efficient strategy to carry out qual. and quant. analyses of the essential oils.

L4 ANSWER 30 OF 35 CAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1992:17927 CAPLUS

DOCUMENT NUMBER: 116:17927

TITLE: "Combination of mass spectrometry and site-specific NMR isotope analyses in the characterization of amino acids"

AUTHOR(S): *Vallet, Claude; Arendt, Margaretha; Mabon, Francoise; Naulet, Norbert; Martin, Gerard J.*

CORPORATE SOURCE: Lab. RMN React. Chim., Univ. Nantes, Nantes, 44072, Fr.

SOURCE: **Journal of the Science of Food and Agriculture (1991), 56(2), 167-85**

CODEN: JSFAAE; ISSN: 0022-5142

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Exptl. strategies were developed that make amino acid probes accessible to the NMR study of site-specific natural isotope fractionation. A multi-isotope approach, based on combined mass spectrometry detn. of H, C, and N overall isotope contents and on ²H-NMR detn. of site-specific H, C, and N isotope ratios, shows that relatively wide ranges of variation are exhibited by the isotopic parameters of glutamic acid, aspartic acid, alanine, proline, and lysine samples from different origins. Moreover, relatively large deviations with respect to a random distribution of ²H among the mol. sites are quantified and compared. A noticeable enantiomeric imbalance at the methylenic site adjacent to the chiral center also is detected in natural samples of L-glutamic and L-aspartic acids in particular. The results are analyzed in terms of filiation criteria and technol. effects. It is shown in particular that the C3 or C4 metabolic origin of the raw materials utilized in fermn. processes can be recognized. Principal component analyses involving the 2 mean isotopic variables .delta.¹³C and .delta.¹⁵N and the 3 site-specific variables (D/H)_z, (D/H)_{beta}, and (D/H)₇ assocd. with positions .alpha., .beta., and .gamma. of glutamic acids, for example, are helpful for interpreting the main discriminating factors. This approach provides the basis for new applications to origin recognition of fundamental constituents and metabolites of plant or animal species.

L4 ANSWER 31 OF 35 CAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1991:578526 CAPLUS

DOCUMENT NUMBER: 115:178526

TITLE: "Determination of site-specific carbon isotope ratios at natural abundance by carbon-13 nuclear magnetic resonance spectroscopy"

AUTHOR *Caer, Valerie; Trierweiler, Michel; Martin, Gerard J.; Martin, Maryvonne L.*

CORPORATE SOURCE: Lab. RMN React. Chim., Univ. Nantes, Nantes, F-44072, Fr.

SOURCE: **Analytical Chemistry (1991), 63(20), 2306-13**

CODEN: ANCHAM; ISSN: 0003-2700

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Site-specific natural isotope fractionation of H studied by ²H NMR (SNIF-NMR) spectroscopy is a powerful source of information on H pathways occurring in biosyntheses in natural conditions. The potential of the C counterpart of this method was investigated and compared. Three typical mol. species, EtOH, HOAc, and vanillin, were considered. By taking into account the requirements of quant. ¹³C NMR, appropriate exptl. procedures were defined and the repeatability and reproducibility of the isotope

ratio detns. were checked under different conditions. The C version of the SNIF-NMR method can detect small differences in the ^{13}C content of the Et fragment of EtOH from different botanical or synthetic origins. The results agree with mass spectrometry detns. of the overall C isotope ratios. Deviations with respect to a statistical distribution of ^{13}C were detected in the case of HOAc and vanillin. However, since the method is very sensitive to several kinds of systematic error, only a relative significance can be attached at present to the internal parameters directly accessible. Isotope-diln. expts. were carried out to check the consistency of the results. In the present state of exptl. accuracy, the ^{13}C NMR method is of more limited potential than ^2H SNIF- NMR spectroscopy. However, it may provide complementary information. It is particularly efficient for detecting and quantifying adulterations that aim to mimic the overall ^{13}C content of a natural compd. by adding a selectively enriched species to a less expensive substrate from a different origin.

L4 ANSWER 32 OF 35 CAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1991:171005 CAPLUS

DOCUMENT NUMBER: 114:171005

TITLE: Authentication of fragrances and perfumes by nuclear magnetic resonance and isotope-ratio mass spectrometry.

AUTHOR(S): Martin, Gerard J.; Hanneguelle, Sophie; Remaud, Gerald

CORPORATE SOURCE: Lab. React. Chim., Univ. Nantes, Nantes, 44072, Fr.

SOURCE: Parfums, Cosmetiques, Aromes (1990), 94, 95-100, 105-9

CODEN: PCARDV; ISSN: 0337-3029

DOCUMENT TYPE: Journal; General Review

LANGUAGE: French

AB A review of 18 refs.

L4 ANSWER 33 OF 35 CAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1986:551610 CAPLUS

DOCUMENT NUMBER: 105:151610

TITLE: "Food quality control and studies on human nutrition by mass spectrometric and nuclear magnetic resonance isotope ratio determination"

AUTHOR(S): Schmidt, H. L.

CORPORATE TU Muenchen, Freising-Weihenstephan, D-8050, Fed. Rep. Ger.

SOURCE: Fresenius' Zeitschrift fuer Analytische Chemie (1986), 324(7), 760-6

CODEN: ZACFAU; ISSN: 0016-1152

DOCUMENT TYPE: Journal; General Review

LANGUAGE: English

AB A review with 46 refs. on the detn. of stable isotope ratios in food by NMR and mass spectrometry to det. the origin of food components, to detect adulteration, and to trace nutrient metab. in humans.

L4 ANSWER 34 OF 35 CAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1982:180634 CAPLUS

DOCUMENT NUMBER: 96:180634

TITLE: "A new method for the identification of the origin of natural products. Quantitative deuterium NMR at the natural abundance level applied to the characterization of anetholes"

AUTHOR(S): *Martin, G. J.; Martin, M. L.; Mabon, F.; Bricout, J.*

CORPORATE SOURCE: Lab. Chim. Org. Phys., CNRS, Nantes, (F) 44072, Fr.

SOURCE: **Journal of the American Chemical Society** (1982), 104(9), 2658-9

CODEN: JACSAT; ISSN: 0002-7863

DOCUMENT TYPE: Journal

LANGUAGE: English

AB A new method for the characterization of the origin of natural products is proposed and illustrated in the case of various anethole samples obtained from fennel, Chinese anise, and chem. synthesis. The method is based on the detection of very spectacular differences in the internal distribution of D at the natural abundance level by means of quant. ^2H NMR. In particular it is capable of distinguishing samples from different origins even when their D/H contents obtained by mass spectroscopy are equal.

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L5 ANSWER 1 OF 53 CAPLUS COPYRIGHT 2003 ACS on STN

TI Chemometric determination of the geographical origin of cow milk using ICP-OES data and isotopic ratios: a preliminary study

L5 ANSWER 2 OF 53 CAPLUS COPYRIGHT 2003 ACS on STN

TI Official methods based on stable isotope techniques for analysis of food. Ten years' of European experience

L5 ANSWER 3 OF 53 CAPLUS COPYRIGHT 2003 ACS on STN

TI Characterization of animal products according to geographic origin and feeding diet using nuclear magnetic resonance and isotope ratio mass spectrometry: cow milk

L5 ANSWER 4 OF 53 CAPLUS COPYRIGHT 2003 ACS on STN

TI Online determination of $^2\text{H}/^1\text{H}$ and $^{13}\text{C}/^{12}\text{C}$ isotope ratios of cinnamaldehyde from different sources using gas chromatography isotope ratio mass spectrometry

L5 ANSWER 5 OF 53 CAPLUS COPYRIGHT 2003 ACS on STN

TI Isotope ratio analysis by HRGC-MS of monoterpene hydrocarbons from citrus essential oils

L5 ANSWER 6 OF 53 CAPLUS COPYRIGHT 2003 ACS on STN

TI Identification of the substance origin marked with deuterated water by isotope ratio mass spectrometry

L5 ANSWER 7 OF 53 CAPLUS COPYRIGHT 2003 ACS on STN

TI Authentication analysis of caffeine-containing foods via elemental analysis combustion/pyrolysis isotope ratio mass spectrometry (EA-C/P-IRMS)

L5 ANSWER 8 OF 53 CAPLUS COPYRIGHT 2003 ACS on STN

TI Isotope ratio analysis by HR-GC-MS of monoterpene hydrocarbons from citrus essential oils

L5 ANSWER 9 OF 53 CAPLUS COPYRIGHT 2003 ACS on STN

TI Stable isotope ratio analysis for authentication of lamb meat

L5 ANSWER 10 OF 53 CAPLUS COPYRIGHT 2003 ACS on STN

TI Multielement, multicomponent, and multisite isotopic profiling for food and beverage authentication

L5 ANSWER 11 OF 53 CAPLUS COPYRIGHT 2003 ACS on STN

TI Isotope fingerprinting: tracing the origin of products

L5 ANSWER 12 OF 53 CAPLUS COPYRIGHT 2003 ACS on STN

TI Isotope ratio analysis by GC-MS and its application to citrus essential oils

L5 ANSWER 13 OF 53 CAPLUS COPYRIGHT 2003 ACS on STN

TI Authentication of Natural Vanilla Flavorings: Isotopic Characterization Using Degradation of Vanillin into Guaiacol

L5 ANSWER 14 OF 53 CAPLUS COPYRIGHT 2003 ACS on STN

TI Differentiation of the geographical origin of durum wheat semolina samples on the basis of isotopic composition

L5 ANSWER 15 OF 53 CAPLUS COPYRIGHT 2003 ACS on STN

TI Origin assessment of green coffee (*Coffea arabica*) by multi-element stable isotope analysis of caffeine

L5 ANSWER 16 OF 53 CAPLUS COPYRIGHT 2003 ACS on STN

TI Tequila Authenticity Assessment by Headspace SPME-HRGC-IRMS Analysis of $^{13}\text{C}/^{12}\text{C}$ and $^{18}\text{O}/^{16}\text{O}$ Ratios of Ethanol

L5 ANSWER 17 OF 53 CAPLUS COPYRIGHT 2003 ACS on STN

TI Chemistry of Archaeological Animal Fats

L5 ANSWER 18 OF 53 CAPLUS COPYRIGHT 2003 ACS on STN

TI Authenticity assessment of guarana products (*Paullinia cupana*) by caffeine isotope analysis

L5 ANSWER 19 OF 53 CAPLUS COPYRIGHT 2003 ACS on STN

TI Authenticity Assessment of Estragole and Methyl Eugenol by On-Line Gas Chromatography-Isotope Ratio Mass Spectrometry

L5 ANSWER 20 OF 53 CAPLUS COPYRIGHT 2003 ACS on STN

TI Isotope ratio by HRGC-MS of Citrus junos Tanaka (Yuzu) essential oils: m/z 137/136 of terpene hydrocarbons

L5 ANSWER 21 OF 53 CAPLUS COPYRIGHT 2003 ACS on STN

TI High precision isotope ratio fingerprinting of ethanol and other commercial molecules and materials

L5 ANSWER 22 OF 53 CAPLUS COPYRIGHT 2003 ACS on STN

TI Characterization of lead glazes and lead leaching properties of glazed ceramics from the Solis Valley, Mexico using inductively coupled plasma- mass spectrometry and diffuse reflectance Fourier transform IR spectroscopy: Are we what we eat out of?

L5 ANSWER 23 OF 53 CAPLUS COPYRIGHT 2003 ACS on STN

TI Use of SNIF-NMR and IRMS in combination with chemometric methods for the determination of chaptalization and geographical origin of wines (the example of Slovenian wines)

L5 ANSWER 24 OF 53 CAPLUS COPYRIGHT 2003 ACS on STN

TI Flavor Authenticity Studies by $2\text{H}/1\text{H}$ Ratio Determination Using On-line Gas Chromatography Pyrolysis Isotope Ratio Mass Spectrometry

L5 ANSWER 25 OF 53 CAPLUS COPYRIGHT 2003 ACS on STN

TI Authenticity control of aromatic substances. Gas chromatographic isotope ratio-mass spectrometry for the determination of $2\text{H}/1\text{H}$ -ratios of benzaldehyde in food

- L5 ANSWER 26 OF 53 CAPLUS COPYRIGHT 2003 ACS on STN
TI The potential of multielement stable isotope analysis for regional origin assignment of butter
- L5 ANSWER 27 OF 53 CAPLUS COPYRIGHT 2003 ACS on STN
TI Development of gas chromatography-isotope ratio mass spectrometry (GCIRMS) as an ancillary technique for tracking, monitoring and determination of the origin of hydrocarbon spills in the environment
- L5 ANSWER 28 OF 53 CAPLUS COPYRIGHT 2003 ACS on STN
TI Incorporation of ^{13}C -labeled coniferyl alcohol into developing Ginkgo biloba L. lignin revealed by analytical pyrolysis and CuO oxidation in combination with isotope ratio monitoring-gas chromatography-mass spectrometry
- L5 ANSWER 29 OF 53 CAPLUS COPYRIGHT 2003 ACS on STN
TI Analytical authentication of natural products
- L5 ANSWER 30 OF 53 CAPLUS COPYRIGHT 2003 ACS on STN
TI Site-specific isotope effects and origin inference
- L5 ANSWER 31 OF 53 CAPLUS COPYRIGHT 2003 ACS on STN
TI Analytical pyrolysis of humic substances and dissolved organic matter in aquatic systems: structure and origin
- L5 ANSWER 32 OF 53 CAPLUS COPYRIGHT 2003 ACS on STN
TI Multielement isotope ratio analysis for detection of authenticity of natural substances
- L5 ANSWER 33 OF 53 CAPLUS COPYRIGHT 2003 ACS on STN
TI Forensic studies by EA-IRMS
- L5 ANSWER 34 OF 53 CAPLUS COPYRIGHT 2003 ACS on STN
TI Examining the origin of melatonin from a "natural" source by isotope ratio mass spectrometry with liquid chromatographic introduction
- L5 ANSWER 35 OF 53 CAPLUS COPYRIGHT 2003 ACS on STN
TI Comparison of bullet alloys by chemical analysis: use of ICP-MS method
- L5 ANSWER 36 OF 53 CAPLUS COPYRIGHT 2003 ACS on STN
TI Detection of Exogenous Sugars or Organic acids Addition in Pineapple Juices and Concentrates by ^{13}C IRMS Analysis
- L5 ANSWER 37 OF 53 CAPLUS COPYRIGHT 2003 ACS on STN
TI Assignment of raw material and authentication of spirits by gas chromatography, hydrogen-, and carbon-isotope ratio measurements. Part 1. Analytical methods and results of a study of commercial products
- L5 ANSWER 38 OF 53 CAPLUS COPYRIGHT 2003 ACS on STN
TI High-precision position-specific isotope analysis
- L5 ANSWER 39 OF 53 CAPLUS COPYRIGHT 2003 ACS on STN
TI Application of ^2H SNIF-NMR and ^{13}C SIRA-MS Analyses to Maple Syrup: Detection of Added Sugars
- L5 ANSWER 40 OF 53 CAPLUS COPYRIGHT 2003 ACS on STN
TI Stable isotope ratio analysis by headspace-GC-IRMS - a contribution for the analysis of alcoholic beverages
- L5 ANSWER 41 OF 53 CAPLUS COPYRIGHT 2003 ACS on STN
TI Investigation of the sorbitol content of wines and an assessment of its authenticity using stable isotope ratio mass spectrometry

L5 ANSWER 42 OF 53 CAPLUS COPYRIGHT 2003 ACS on STN
TI Inter- and intramolecular isotope correlations in organic compounds as a criterion for authenticity identification and origin assignment

L5 ANSWER 43 OF 53 CAPLUS COPYRIGHT 2003 ACS on STN
TI Deuterium, carbon and nitrogen isotopic analysis of natural and synthetic caffeine. Authentication of coffees and coffee extracts

L5 ANSWER 44 OF 53 CAPLUS COPYRIGHT 2003 ACS on STN
TI Combination of mass spectrometry and site-specific NMR isotope analyses in the characterization of amino acids

L5 ANSWER 45 OF 53 CAPLUS COPYRIGHT 2003 ACS on STN
TI Enantiomeric distribution and $^{13}\text{C}/^{12}\text{C}$ isotope ratio determination of γ -lactones: appropriate methods for the differentiation between natural and non-natural flavors?

L5 ANSWER 46 OF 53 CAPLUS COPYRIGHT 2003 ACS on STN
TI Determination of site-specific carbon isotope ratios at natural abundance by carbon-13 nuclear magnetic resonance spectroscopy

L5 ANSWER 47 OF 53 CAPLUS COPYRIGHT 2003 ACS on STN
TI Isotope mass spectrometry. Principles and applications

L5 ANSWER 48 OF 53 CAPLUS COPYRIGHT 2003 ACS on STN
TI Determination of origin of acetic acid in alcohol vinegars. 1

L5 ANSWER 49 OF 53 CAPLUS COPYRIGHT 2003 ACS on STN
TI The IDA-80 measurement evaluation program on mass spectrometric isotope dilution analysis of uranium and plutonium.

Volume III: Compilation of evaluation data

L5 ANSWER 50 OF 53 CAPLUS COPYRIGHT 2003 ACS on STN
TI Searching for materials of ancient mirrors. Lead isotope ratio method

L5 ANSWER 51 OF 53 CAPLUS COPYRIGHT 2003 ACS on STN
TI A new method for the identification of the origin of natural products. Quantitative deuterium NMR at the natural abundance level applied to the characterization of anetholes

L5 ANSWER 52 OF 53 CAPLUS COPYRIGHT 2003 ACS on STN
TI Intramolecular carbon-13/carbon-12 isotope ratios of acetic acid of biological and synthetic origin

L5 ANSWER 53 OF 53 CAPLUS COPYRIGHT 2003 ACS on STN
TI New evidence of the origin of pre-Cambrian carbon

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L6 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1997:135111 CAPLUS

DOCUMENT NUMBER: 126:235451

TITLE: High-precision position-specific isotope analysis

AUTHOR(S): Corso, Thomas N.; Brenna, J. Thomas

CORPORATE SOURCE: Div. Nutritional Sci., Cornell Univ., Ithaca, NY, 14853, USA

SOURCE: Proceedings of the National Academy of Sciences of the United States of America (1997), 94(4), 1049-1053

CODEN: PNASA6; ISSN: 0027-8424

PUBLISHER: National Academy of Sciences

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Intramol. carbon isotope distributions reflect details of the origin of org. compds. and may record the status of complex systems, such as environmental or physiol. states. A strategy is reported here for high-precision detn. of $^{13}\text{C}/^{12}\text{C}$ ratios at specific positions in org. compds. sepd. from complex mixts. Free radical fragmentation of Me palmitate, a test compd., is induced by an open tube furnace. Two series of peaks corresponding to bond breaking from each end of the mol. are analyzed by isotope ratio mass spectrometry and yield precisions of $\text{SD}(\delta\text{-}^{13}\text{C}) < 0.4\text{ permill.}$ Isotope labeling in the carboxyl, terminal, and Me positions demonstrates the absence of rearrangement during activation and fragmentation. Negligible isotopic fractionation was obsd. as degree of fragmentation was adjusted by changing pyrolysis temp. $[1\text{-}^{13}\text{C}]\text{methyl palmitate}$ with overall $\delta\text{-}^{13}\text{C} = 4.06\text{ permill.}$, yielded values of $+457\text{ permill.}$ for the carboxyl position, in agreement with expectations from the diln., and an av. of -27.95 permill. for the rest of the mol., corresponding to -27.46 permill. for the olefin series. These data demonstrate the feasibility of automated high-precision position-specific anal. of C for mols. contained in complex mixts.

L6 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1994:639573 CAPLUS

DOCUMENT NUMBER: 121:239573

TITLE: The origin and distribution of the E1 strength over low-lying states in well-deformed nuclei

AUTHOR(S): Soloviev, V. G.; Sushkov, A. V.

CORPORATE SOURCE: Joint Institute Nuclear Research, Dubna, Russia

SOURCE: Yadernaya Fizika (1994), 57(8), 1375-85

CODEN: IDFZA7; ISSN: 0044-0027

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The energies and wave functions of the $K\pi = 0^-$ and 1^- states in ^{158}Gd , $^{162,164}\text{Dy}$ and ^{168}Er are calcd. in the RPA by taking the isoscalar and isovector particle-hole and particle-particle octupole and isovector particle-hole dipole interactions into account. The inclusion of the isovector dipole interaction in addn. to the octupole ones leads to the shift of the largest part of the E1 strength from low-lying states to the GDR. The origin of the E1 strength in the low-energy region is explained as an effect on the quadrupole equil. deformation and isoscalar octupole and isovector dipole interactions. The total E1 strength for $K\pi = 0^-$ states is 3-4 times as large as for $K\pi = 1^-$ states at excitation energies below 4 MeV. The fragmentation of the one-phonon $K\pi = 0^-$ and 1^- states in ^{164}Dy and ^{168}Er due to coupling with two-phonon configuration is calcd. The $B(E1)$ values for the first $K\pi = 0^-$ states are 3-5 times as large as the exptl. ones. The concn. of the E1 strength over $K\pi = 0^-$ states at energies 2.6-3.5 MeV in ^{168}Er and 3.6-3.9 MeV in ^{164}Dy is predicted.